

Microscopic view of hydrogen adsorption in size-variant nano-clay materials

Wednesday, 4 June 2025 11:30 (15 minutes)

Hydrogen is the carbon-free fuel par excellence because its combustion emits only water. Research has focused on H₂ storage in lightweight materials for the needs of vehicles, excluding clays due to their weight. But large-scale terrestrial storage for industrial applications does not require the same specifications. In this context, clay minerals offer several interesting properties, such as large surface area, low cost, global abundance and environmental safety.

We investigate, at the microscopic level, H₂ adsorption on synthetic 2:1 trioctahedral smectites of nanometric dimensions, specifically Laponite, and its precursor, pre-Laponite. Our aim is to understand the higher H₂ sorption capacity of pre-Laponite, combining adsorption isotherm measurements, elastic and inelastic neutron scattering experiments and Grand Canonical Monte Carlo (GCMC) simulations.

The adsorption isotherms at 40 K, up to 1 bar, are fitted with a Langmuir contribution and a smoothest one. GCMC simulations show that the Langmuir model, accounting for the strongest binding sites, describes adsorption within the interlayer, as confirmed by small angle neutron scattering. Inelastic neutron scattering experiments were undertaken to probe the para-to-ortho rotational transition of H₂, the energy of which is highly sensitive to its environment. At 40K, two adsorption sites are identified in the interlayer, with orientational potential wells of about 80K and 1300K, respectively. Based on wide angle neutron scattering analysis, the second site would be situated above the hexagonal cavity defined by Si tetrahedra. Quantum sieving effects were also evidenced comparing D₂ and H₂ adsorption. The highest adsorption in pre-Laponite compared to Laponite is attributed to the slightly more open interlayer space (sheet-to-sheet distance is 1 nm in pre-Laponite and 0.97 nm in Laponite).

The perspective of these results is the fine modulation of the interlayer space to optimize the storage of hydrogen in clays at low temperature and beyond, under pressure, at room temperature.

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Session Classification: Contributed talks